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The approximate regularization of index-2 differential-algebraic problems

Yuhe Ren

School of Mathematical Sciences, University of Bath, Bath BA2 7AY, UK

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Abstract

The approximate regularization method is introduced for the solution of index-2 Hessenberg systems of differential-algebraic equations. This approach is based on using a Taylor-series-type method, which results in a singular perturbation ordinary differential systems. For linear problems, it is shown that this approach is stable. To compare with a partial regularization, the approximate regularization appears to be promising.

Keywords: Differential-algebraic equation; Regularization

AMS classification: 65L05; 65L10

1. Introduction

In this paper, we consider index-2 differential-algebraic problem

$$x' = f(x, y, t), \tag{1a}$$

$$0 = g(x, t), \tag{1b}$$

where $g_x f_y$ is assumed to be nonsingular in a neighborhood of the solution, and assume consistent initial values x_0, y_0.

Differentiating (1a), we get

$$x'' = f_x x' + f_y y' + f_t.$$

In order to compute y' we differentiate (1b) twice:

$$0 = g_x x' + g_t,$$

$$0 = (g_{xx} x' + g_{xt}) x' + g_x x'' + (g_{tx} x' + g_{tt}).$$

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This yields

$$0 = g_{xx}f^2 + g_{xt}f + g_x(f_x f + f_y y' + f_t) + g_{xt}f + g_{tt},$$

or equivalently

$$-(g_x f_y)y' = g_{xx}f^2 + g_x f_x f + g_x f_t + 2g_{xt}f + g_{tt}. \tag{2}$$

However, the solution can drift away from both the position and velocity constraints since the differential system is unstable.

If one wishes to view (1) as a reduced-order equation for a perturbed problem, and if the solutions are to be continuous in the perturbation parameter, then the obvious regularization

$$x' = f(x, y, t) \qquad \varepsilon y' = g(x, t)$$

may not be the correct regularization.

One of the most popular techniques for reformulating the constraint equation is due to Baumgarte [3]. For the index-2 system (1), Baumgarte's method replaces the position constraint by a linear combination of the position, velocity constraints,

$$g(x, t) + \gamma \frac{\mathrm{d}}{\mathrm{d}t} g(x, t) = 0, \tag{3}$$

where the constant γ is chosen so that the differential equation for g is stable. Baumgarte's method can be considered to be a regularization of the differential-algebraic equation. As a regularization it has the special property that, unlike many other regularizations, the analytical solution to the Baumgarte stabilization of a DAE is identical to the solution of the original DAE. But the parameter γ in Baumgarte's method is difficult to choose [2].

Lötstedt [11] considers a partial regularization,

$$x' = f(x, y, t, \varepsilon), \tag{4a}$$

$$\varepsilon y = g(x, t, \varepsilon). \tag{4b}$$

This system is a singular singular-perturbation problem [7] since for $\varepsilon > 0$, it is an index-1 DAE, while for $\varepsilon = 0$ it is index-2.

Differentiating (4b) and using (4a), we get an ODE system

$$x' = f(x, y, t, \varepsilon), \tag{5}$$

$$\varepsilon y' = g_x f + g_t \tag{6}$$

and the corresponding reduced-order problem

$$x' = f(x, y, t, 0), \tag{7}$$

$$0 = g_x f + g_t. \tag{8}$$

Note that the solutions of the original index-2 DAE (1) are solutions of the index-1 DAE (8), and that the solutions of (4) are solutions of (6).

Assuming that $g_x f_y$ is negative-definite in a neighborhood of the solution of the initial problem, an analysis can be carried out for these systems that is similar to that for index-1 systems. If $||g(x(0), 0, \varepsilon)|| = O(\varepsilon)$, then uniform asymptotic expansions exist. If, however, $||g(x(0), 0, \varepsilon)|| = O(1)$, which would be the case if $g(x(0), 0, 0) \neq 0$, then there is a term which has a distributional limit as $\varepsilon \to 0^+$.

In Section 2, we propose an approximate regularization method for the solution of index-2 Hessenberg systems of DAEs. In Section 3, the stability of the regularized system is investigated and the asymptotic solutions are obtained by using the asymptotic approach. In Section 4, the numerical results are presented to compare with a partial regularization approach. The conclusions are in Section 5.

2. Approximate regularization technique

Here we consider the solution of the constraint equation (1). Consider (x_{n+1}, t_{n+1}), where $x_{n+1} = x_n + hx_n' + \frac{1}{2}h^2 x_n'' + O(h^3)$ and $t_{n+1} = t_n + h$. Since

$$x_n' = \frac{x_{n+1} - x_n}{h} - \frac{h}{2}x_n'' + O(h^2)$$

and the truncation error for Newton's method is also $O(h^2)$, we ignore the $O(h^3)$ term in x_{n+1}. Actually, the Taylor series for x_{n+1} is only considered for solving constraint equations. We will solve the original $x' = f$ with high-order accuracy in time by a BDF code DASSL [4] as we can see later.

Let

$$0 = g(x_{n+1}, t_{n+1}) = g(x_n + hx_n' + \tfrac{1}{2}h^2 x_n'' + O(h^3), t_n + h). \tag{9a}$$

The Newton method is applied to (9a) for solving (x_n, t_n), thus,

$$g(x_n, t_n) + g_x(x_n, t_n)(hx_n' + \tfrac{1}{2}h^2 x_n'') + hg_t(x_n, t_n) = 0. \tag{10}$$

To adjust the direction of y such that $hx' + \frac{1}{2}h^2 x''$ is the Newton descent direction in (9a), since

$$x' = f(x, y, t), \tag{11}$$

$$x'' = f_x x' + f_y y' + f_t, \tag{12}$$

substituting (11) and (12) into (10), we get

$$g + g_x[hf + \tfrac{1}{2}h^2(f_x f + f_y y' + f_t)] + hg_t = 0.$$

The regularized ordinary differential system is

$$x' = f(x, y, t), \tag{13a}$$

$$-\tfrac{1}{2}h^2 g_x f_y y' = g + hg_x f + \tfrac{1}{2}h^2 g_x f_x f + \tfrac{1}{2}h^2 g_x f_t + hg_t. \tag{13b}$$

For $h = 0$, system (13) is the original differential-algebraic problem (1).

3. Stability and asymptotic solutions

Consider the index-2 DAE

$$x' = Ax + By + q(t), \tag{14a}$$

$$0 = Cx + r(t), \tag{14b}$$

where A, B and C are smooth functions of t, $0 \leqslant t \leqslant 1$, $A(t) \in \mathbb{R}^{n_x \times n_x}$, $B(t) \in \mathbb{R}^{n_x \times n_y}$, $C(t) \in \mathbb{R}^{n_y \times n_x}$, $n_y \leqslant n_x$ and CB is nonsingular for each t. The inhomogeneities are $q(t) \in \mathbb{R}^{n_x}$ and $r(t) \in \mathbb{R}^{n_y}$.

As in [1], since CB is nonsingular, B has full rank. Hence, there exists a smooth, bounded matrix function $R(t) \in \mathbb{R}^{(n_x - n_y) \times n_x}$, whose linearly independent rows form a basis for the null space of B. The existence of such R can be obtained from [5]. Further, R can be taken to be orthonormal. Thus, for each t, $0 \leqslant t \leqslant 1$,

$$RB = 0.$$

Define new variables

$$w = Rx.$$

Then, using (14b), the inverse transformation is given by

$$x = \begin{pmatrix} R \\ C \end{pmatrix}^{-1} \begin{pmatrix} w \\ -r \end{pmatrix} \equiv Sw - Fr, \tag{15}$$

where $S(t) \in \mathbb{R}^{n_x \times (n_x - n_y)}$ satisfies

$$RS = I, \qquad CS = 0$$

and

$$F := B(CB)^{-1}.$$

Multiplying (14a) by R, we have

$$Rx' = RAx + Rq.$$

Using (15), we obtain the *essential underlying* ODE (EUODE)

$$w' = (RA + R')Sw + Rq - (RA + R')Fr. \tag{16}$$

If this ODE problem is stable, then the DAE (14) is stable too.

Now, consider the regularization problem (13):

$$x' = Ax + By + q(t), \tag{17a}$$

$$\begin{aligned} -\tfrac{1}{2}h^2(CB)y' = {} & Cx + r + (hC + \tfrac{1}{2}h^2(CA))(Ax + By + q) \\ & + \tfrac{1}{2}h^2 C(A'x + B'y + q') + h(C'x + r'). \end{aligned} \tag{17b}$$

The reduced problem is

$$X' = AX + BY + q(t), \tag{18a}$$

$$0 = CX + r(t). \tag{18b}$$

We will investigate the stability of the approximate regularization problem (17). It is important to obtain a similar essential underlying ODE as mentioned above. Hence, let us set

$$v(t) = y(t) + L(t,h)x(t)$$

or, equivalently,

$$y(t) = v(t) - L(t,h)x(t).$$

Substitute it into (17b),

$$\begin{aligned} -\tfrac{1}{2}h^2(CB)v' = {} & Cx + r + (hC + \tfrac{1}{2}h^2CA - \tfrac{1}{2}h^2(CB)L)((A - BL)x + q) \\ & + \tfrac{1}{2}h^2C((A' - B'L)x + q') + h(C'x + r') - \tfrac{1}{2}h^2(CB)L'x \\ & + (hC + \tfrac{1}{2}h^2CA - \tfrac{1}{2}h^2(CB)L)Bv + \tfrac{1}{2}h^2CB'v. \end{aligned}$$

We choose L which is a solution of the singularly perturbed matrix Riccati equation

$$\tfrac{1}{2}h^2(CB)L' = C + (hC + \tfrac{1}{2}h^2CA - \tfrac{1}{2}h^2(CB)L)(A - BL) + \tfrac{1}{2}h^2C(A' - B'L) + hC'. \tag{19}$$

This implies that v will satisfy the system

$$-\tfrac{1}{2}h^2(CB)v' = hDv + \bar{r}, \tag{20}$$

where

$$D = (C + \tfrac{1}{2}hCA - \tfrac{1}{2}h(CB)L)B + \tfrac{1}{2}hCB',$$

$$\bar{r} = r + hr' + (hC + \tfrac{1}{2}h^2CA - \tfrac{1}{2}h^2(CB)L)q + \tfrac{1}{2}h^2Cq'.$$

From (19), the matrix L has asymptotic expansion [13]

$$L(t,h) \sim \frac{1}{h}L_{-1} + L_0 + hL_1 + \cdots$$

and determine coefficients termwise from the matrix differential equation. Thus,

$$C - CBL_{-1} = 0$$

or

$$L_{-1} = (CB)^{-1}C.$$

Now, we study the stability of the system (20). The leading term of the matrix D is

$$CB - \tfrac{1}{2}(CB)L_{-1}B = \tfrac{1}{2}CB.$$

Hence, we can see that the system (20) is a stable system.

Having found L and v, the vector x will satisfy the system

$$x' = (A - BL)x + Bv + q(t).$$

We introduce a vector u through a new transformation

$$u = x + hHv.$$

Differentiating, we have

$$\begin{aligned} u' &= x' + hH'v + hHv' \\ &= (A - BL)(u - hHv) + Bv + q + hH'v + hHv' \\ &= (A - BL)u + (-h(A - BL)H + B + hH' - 2H(CB)^{-1}D)v + q - \frac{2}{h}H(CB)^{-1}\bar{r}. \end{aligned}$$

We choose H to satisfy the singular perturbed linear matrix system

$$hH' = h(A - BL)H - B + 2H(CB)^{-1}D. \tag{21}$$

We seek a smooth solution $H(t,h)$ with an asymptotic series expansion

$$H(t,h) \sim H_0(t) + hH_1(t) + h^2H_2(t) + \cdots .$$

Equating coefficients successively, we first have

$$H_0 = \tfrac{1}{2}BD^{-1}(CB)$$

and, then we can determine H_j for each $j > 0$. So u will satisfy the system

$$u' = (A - BL)u + q - \frac{2}{h}H(CB)^{-1}\bar{r}.$$

Having found u, v, L and H, we can obtain the asymptotic solutions for x and y,

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} I & -hH \\ -L & I + hLH \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}. \tag{22}$$

To compare with the choice of the parameters in Baumgarte's method which is a sensitive [2], the choice of h is clear. We can choose h to be a stepsize of the integration.

4. Examples

In this section, we test some examples to demonstrate efficiency of the regularized system (13). The DAE code DASSL [4] was used in all examples. Absolute and relative error tolerances were set to 10^{-6}.

Example 1. Consider for $0 \leqslant t \leqslant 1$

$$x_1' = \left(\lambda - \frac{1}{2-t}\right)x_1 + (2-t)\lambda y + \frac{3-t}{2-t}e^t,$$

$$x_2' = \frac{1-\lambda}{t-2}x_1 - x_2 + (\lambda - 1)y + 2e^t,$$

$$0 = (t+2)x_1 + (t^2-4)x_2 - (t^2+t-2)e^t,$$

with $x_1(0) = 1$. Here $\lambda \geqslant 1$ is a parameter. The exact solution is $x_1(t) = x_2(t) = e^t$, and $y(t) = -[e^t/(2-t)]$. Choose

$$R(t) = \lambda^{-1}(1-\lambda, (2-t)\lambda).$$

Then, it can be verified that the essential underlying ODE (16) for the homogeneous problem is

$$u' = -\left(\lambda + \frac{1}{2-t}\right)u$$

with

$$u(0) = \frac{1}{\lambda} + 1.$$

This is a stable initial-value problem. But it can be verified that the ghost ODE which governs the stability of the midpoint scheme is

$$\hat{y}' = \frac{\lambda}{2-t}\hat{y},$$

which is unstable exponentially in λ [1].

Example 2. The nonlinear BVP

$$x_1' = x_3,$$

$$x_2' = x_4,$$

$$x_3' = -y_1 x_1 + e^t(1 + \sin t),$$

$$x_4' = -y_1 x_2 + \frac{1}{1+t}\left(\frac{2}{(1+t)^2} + \sin t\right),$$

$$x_3 x_2^3 + (3x_1 x_2^2 + e^{x_2})x_4 = \frac{e^t}{(1+t)^3} - \frac{3e^t}{(1+t)^4} - \frac{e^{1/(1+t)}}{(1+t)^2},$$

where $x_1(0) = 1$, $x_3(0) = 1$ and $x_1(1) = e$, has the exact solution $x^T = (e^t, (1+t)^{-1}, e^t, -(1+t)^{-2})$, $y_1 = \sin t$. This example was derived by one differentiation of the constraint in the index-3 DAE

$$z_1'' = -y_1 z_1 + e^t(1 + \sin t),$$

Table 1
Errors for Example 2
$h = 10^{-3}$

t	Error in x_1	Error in x_3	Drift	Step size
0.1	$8.7\cdot10^{-5}$	$8.5\cdot10^{-4}$	$4.5\cdot10^{-3}$	$1.1\cdot10^{-3}$
0.5	$3.6\cdot10^{-4}$	$4.9\cdot10^{-4}$	$1.9\cdot10^{-3}$	$2.1\cdot10^{-3}$
1.0	$5.8\cdot10^{-4}$	$2.0\cdot10^{-4}$	$1.0\cdot10^{-3}$	$1.9\cdot10^{-4}$

$h = 10^{-4}$

t	Error in x_1	Error in x_3	Drift	Step size
0.1	$2.4\cdot10^{-5}$	$1.7\cdot10^{-4}$	$4.5\cdot10^{-4}$	$2.7\cdot10^{-4}$
0.5	$3.3\cdot10^{-4}$	$7.2\cdot10^{-4}$	$1.9\cdot10^{-4}$	$8.7\cdot10^{-4}$
1.0	$1.9\cdot10^{-3}$	$2.5\cdot10^{-3}$	$1.0\cdot10^{-4}$	$2.5\cdot10^{-3}$

Table 2
Errors for Example 2: Lötstedt's regularization

ε	t	Error in x_1	Error in x_3	Drift
0.1	0.1	$6.3\cdot10^{-5}$	$1.5\cdot10^{-3}$	$8.0\cdot10^{-3}$
	0.5	$3.5\cdot10^{-3}$	$1.8\cdot10^{-2}$	$4.3\cdot10^{-2}$
	1.0	$2.2\cdot10^{-2}$	$6.1\cdot10^{-2}$	$7.9\cdot10^{-2}$
10^{-2}	0.1	$8.6\cdot10^{-5}$	$1.9\cdot10^{-4}$	$9.7\cdot10^{-4}$
	0.5	$3.8\cdot10^{-4}$	$2.0\cdot10^{-3}$	$4.7\cdot10^{-3}$
	1.0	$2.4\cdot10^{-3}$	$6.6\cdot10^{-3}$	$8.3\cdot10^{-3}$

$$z_2'' = -y_1 z_2 + \frac{1}{1+t}\left(\frac{2}{(1+t)^2} + \sin t\right),$$

$$0 = z_1 z_2^3 + e^{z_2} - \frac{e^t}{(1+t)^3} - e^{1/(1+t)}.$$

In Table 1 we list the errors in x_1 and in x_3 for $h = 10^{-3}$ and 10^{-4}. The accuracy for the constraint is $O(h)$ which is consistent with the analytical result, the constraint is perturbed with $O(h)$ based on the Taylor-series approach. The regularized system is easily solved by DASSL [4]. In Table 2, we also list the results for the partial regularization with $\varepsilon = 10^{-1}, 10^{-2}$. DASSL [4] does not converge for the smaller ε. From the tables we can see that the approximate regularization is better than the partial regularization.

Example 3. The pendulum problem

$$x_1'' = -\lambda x_1,$$

$$x_2'' = -\lambda x_2 - g,$$

$$0 = x_1^2 + x_2^2 - L^2,$$

Table 3
Errors for Example 3

h	Error in x_1	Error in x_3	Drift 1	Drift 2	Step size
10^{-2}	$1.2 \cdot 10^{-3}$	$7.7 \cdot 10^{-5}$	$2.0 \cdot 10^{-4}$	$2.6 \cdot 10^{-5}$	$1.4 \cdot 10^{-2}$
10^{-3}	$3.4 \cdot 10^{-5}$	$7.8 \cdot 10^{-7}$	$1.2 \cdot 10^{-6}$	$2.4 \cdot 10^{-7}$	$1.1 \cdot 10^{-2}$
10^{-4}	$5.1 \cdot 10^{-3}$	$2.3 \cdot 10^{-3}$	$4.0 \cdot 10^{-3}$	$2.6 \cdot 10^{-6}$	$1.7 \cdot 10^{-2}$

Table 4
Errors for Example 3: Lötstedt's regularization

ε	Error in x_1	Error in x_3	Drift 1	Drift 2
10^{-2}	$1.9 \cdot 10^{-1}$	$2.5 \cdot 10^{-2}$	$5.0 \cdot 10^{-2}$	$3.6 \cdot 10^{-2}$
10^{-3}	$2.4 \cdot 10^{-2}$	$2.6 \cdot 10^{-3}$	$5.0 \cdot 10^{-3}$	$3.9 \cdot 10^{-3}$

where (x_1,x_2) are Cartesian coordinates of an infinitesimal ball of unity mass, L is the pendulum length, y is the tension in the bar, and g is the gravitational force. This is an index-3 DAE, which can be converted to an index-2 DAE by one constraint differentiation:

$$
\begin{aligned}
x_1' &= x_3,\\
x_2' &= x_4,\\
x_3' &= -\lambda x_1,\\
x_4' &= -\lambda x_2 - g,\\
0 &= x_1 x_3 + x_2 x_4,
\end{aligned}
$$

where $0 \leqslant t \leqslant$, and initial conditions satisfy $x_2(0) = -\sqrt{L^2 - x_1^2(0)}$.

Consider the IVP with $L=1$, $g=1$, $x_1(0)=1$, $x_3(0)=0$, $x_4(0)=-1$, $\lambda(0)=1$ and $T=1$. We calculate the "drifts",

$$
\begin{aligned}
\text{drift}\,1 &= x_1^2(1) + x_2^2(1) - L^2,\\
\text{drift}\,2 &= x_1(1)x_3(1) + x_2(1)x_4(1),
\end{aligned}
$$

in addition to the errors at $t=T$, based on the "exact" values given in [4]. In Table 3, we list errors in x_1 and in x_3 for $h=10^{-2}, h^{-3}$ and h^{-4}, respectively.

From these errors, it is clear that the errors in the velocity constraint are smaller than the errors in the position constraint. The $h=10^{-3}$ is the best choice for this problem. To compare with the partial regularization, we have tested it for $\varepsilon = 10^{-2}$ and 10^{-3}. The results are given in Table 4. The approximate regularization approach is promising.

5. Conclusions

We have studied the approximate regularization method for the solution of index-2 Hessenberg systems of differential-algebraic equations. We use the Taylor-series-type approach to solve the constraint by Newton's method. The regularized system is a singular perturbation ordinary differential systems. The choice of the parameter h is clear, we can choose it as a step size of the integration. For linear problems, we have shown that the regularized system is stable. The asymptotic solutions can be obtained by using the asymptotic approach while it is a stiff ordinary differential system as the parameter is a very small. We consider only an index-2 DAEs although a similar idea can be applied to an index-3 DAEs. To compare with a partial regularization approach, the approximate regularization appears to be promising.

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